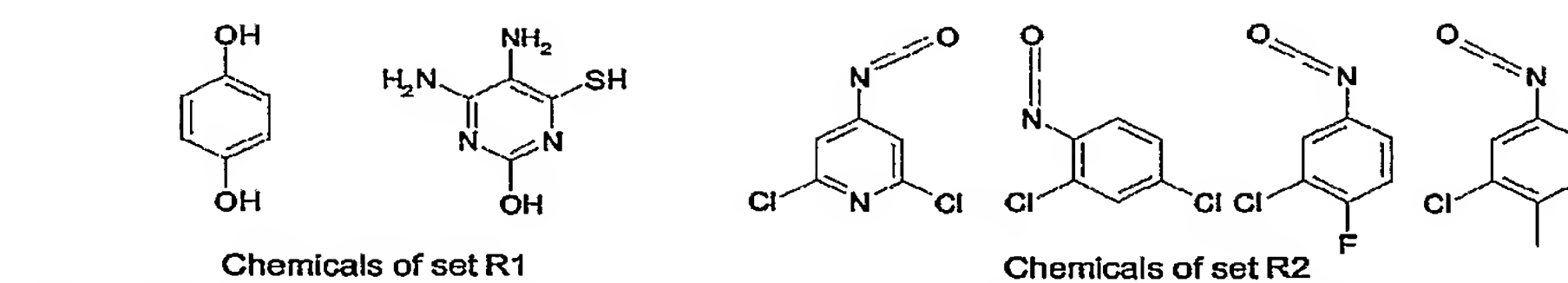
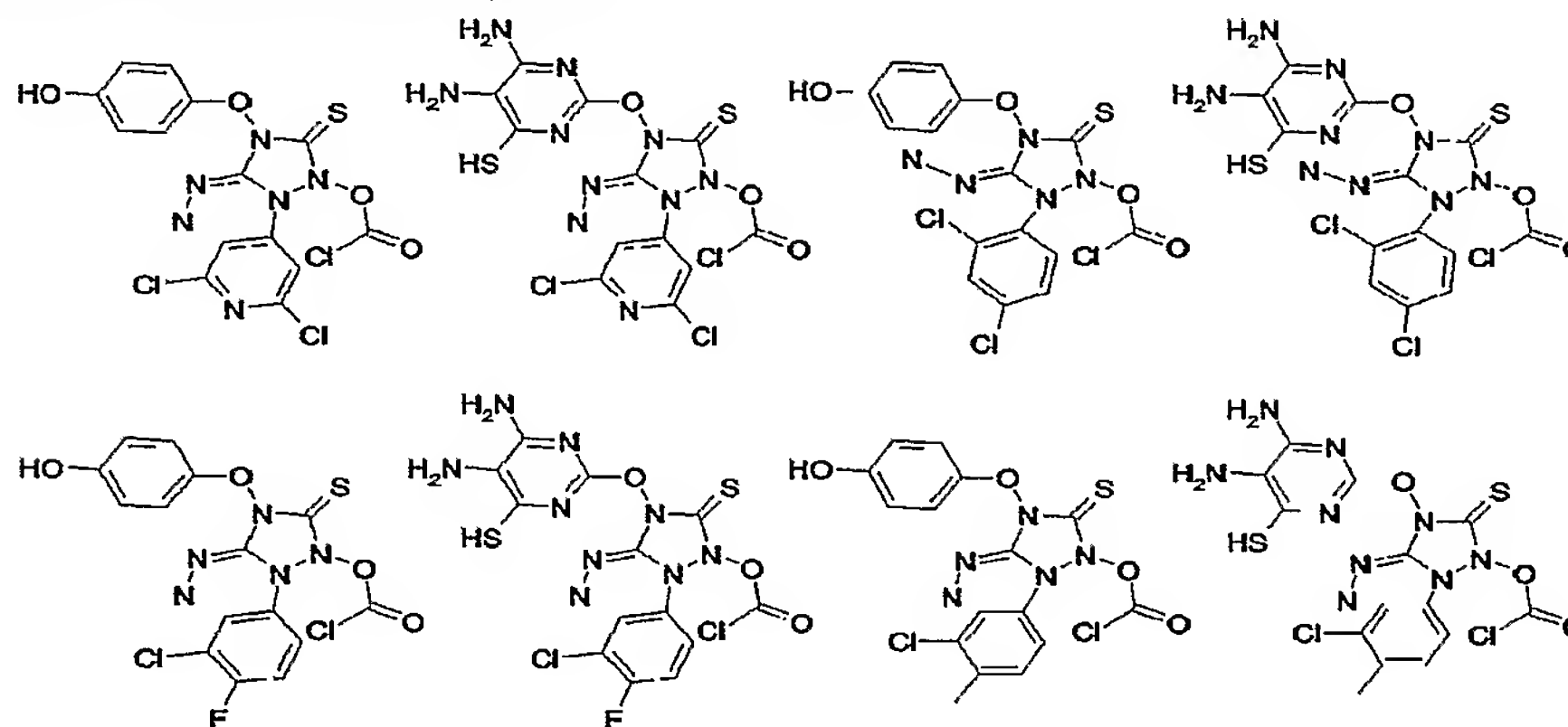
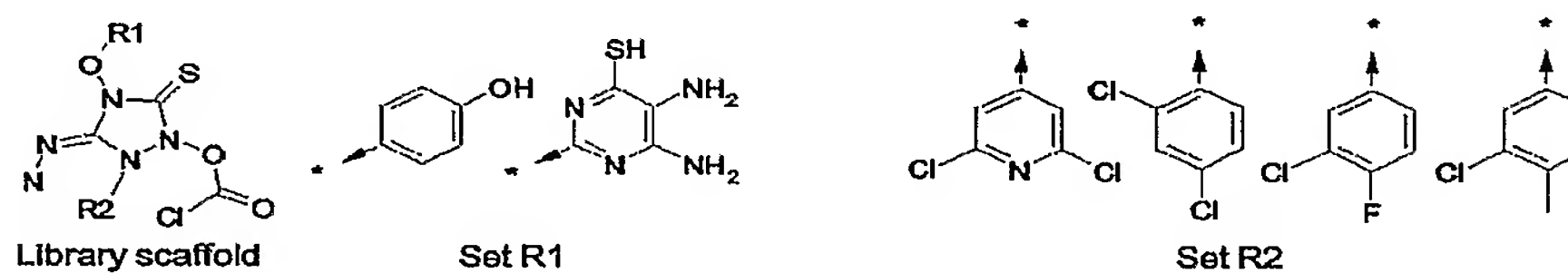


**Figure 1**

Under certain conditions, each chemical in set R1 may react with each chemical in set R2 and yield to the following set of compounds:

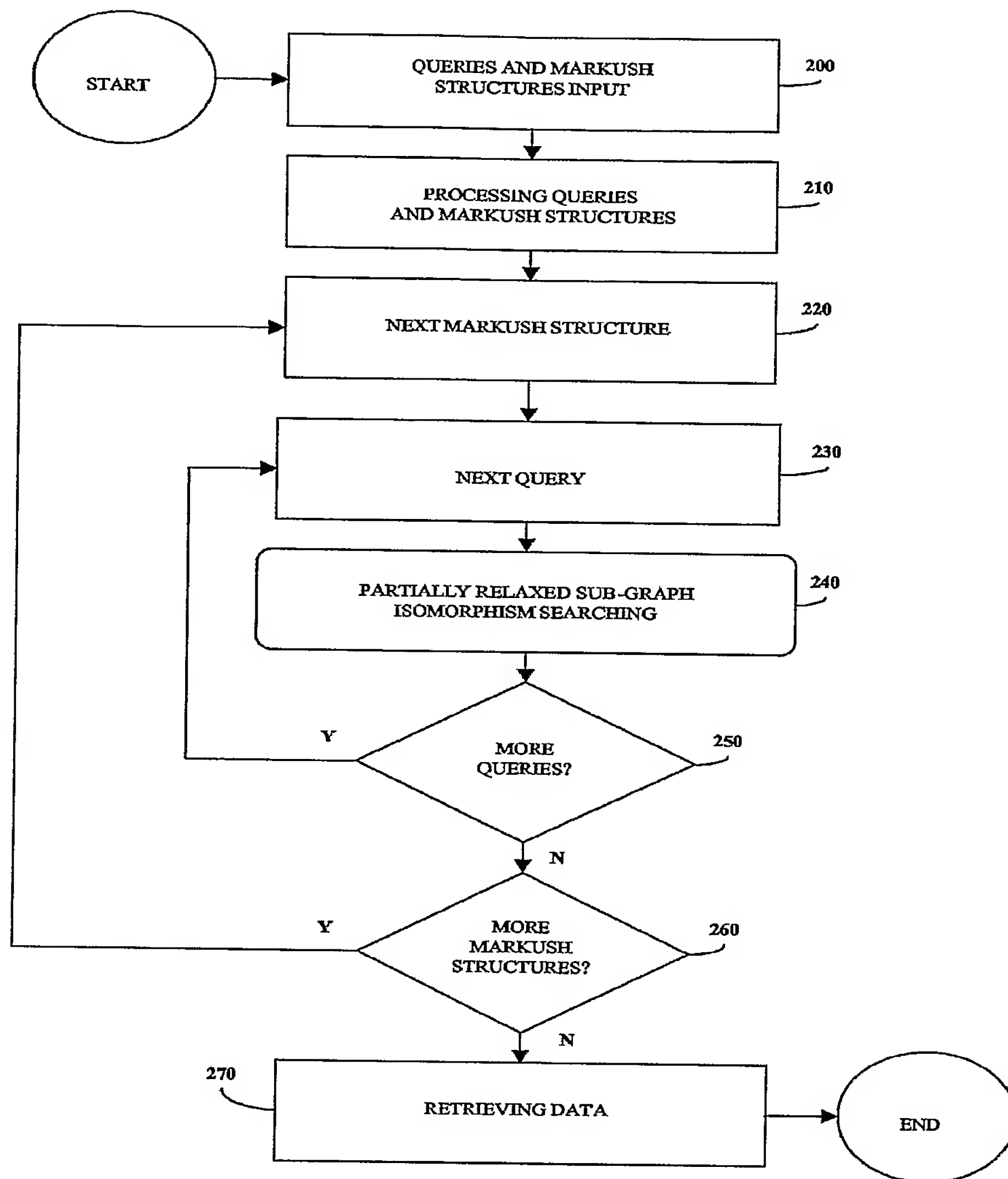


These eight compounds are represented by the following non-enumerated library. This representation is also called Markush representation:



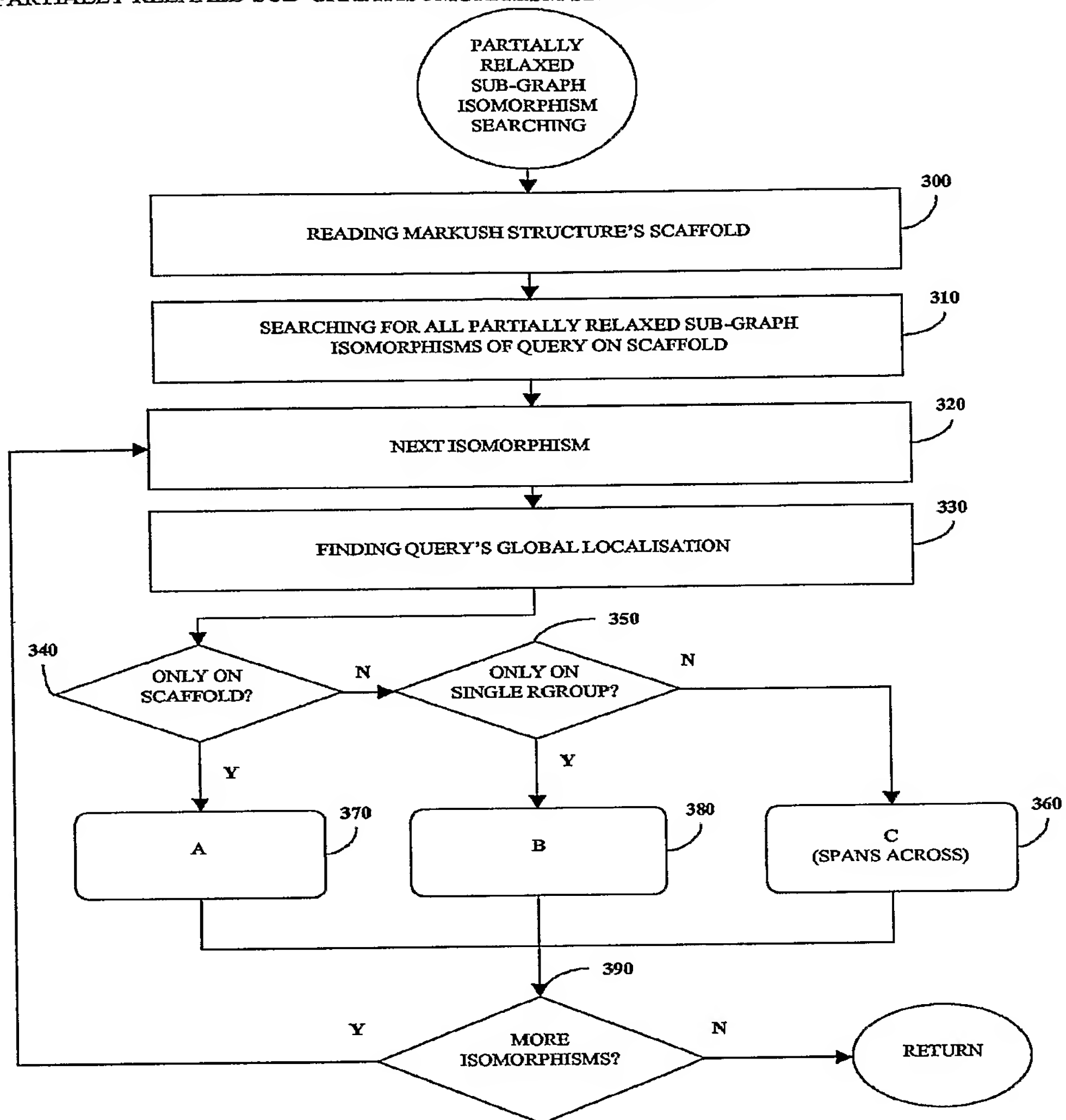
**The Markush representation**

Figure 2



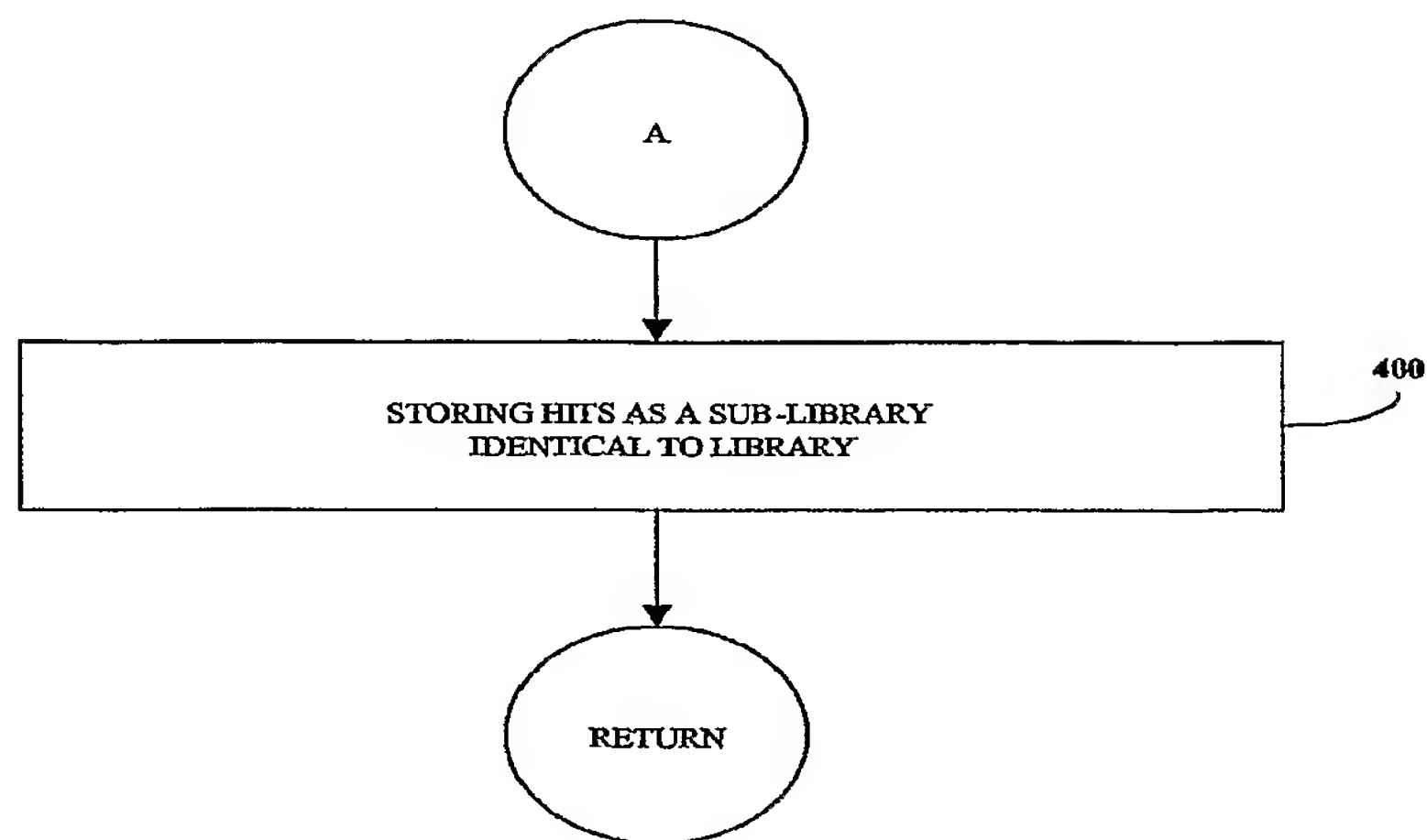
**Figure 3**

SUBROUTINE:  
PARTIALLY RELAXED SUB-GRAPH ISOMORPHISM SEARCHING



**Figure 4**

SUBROUTINE:  
A (QUERY IS LOCATED ONLY ON THE SCAFFOLD)



**Figure 5**

SUBROUTINE:  
B (QUERY IS LOCATED ONLY ON A SINGLE RGROUP)

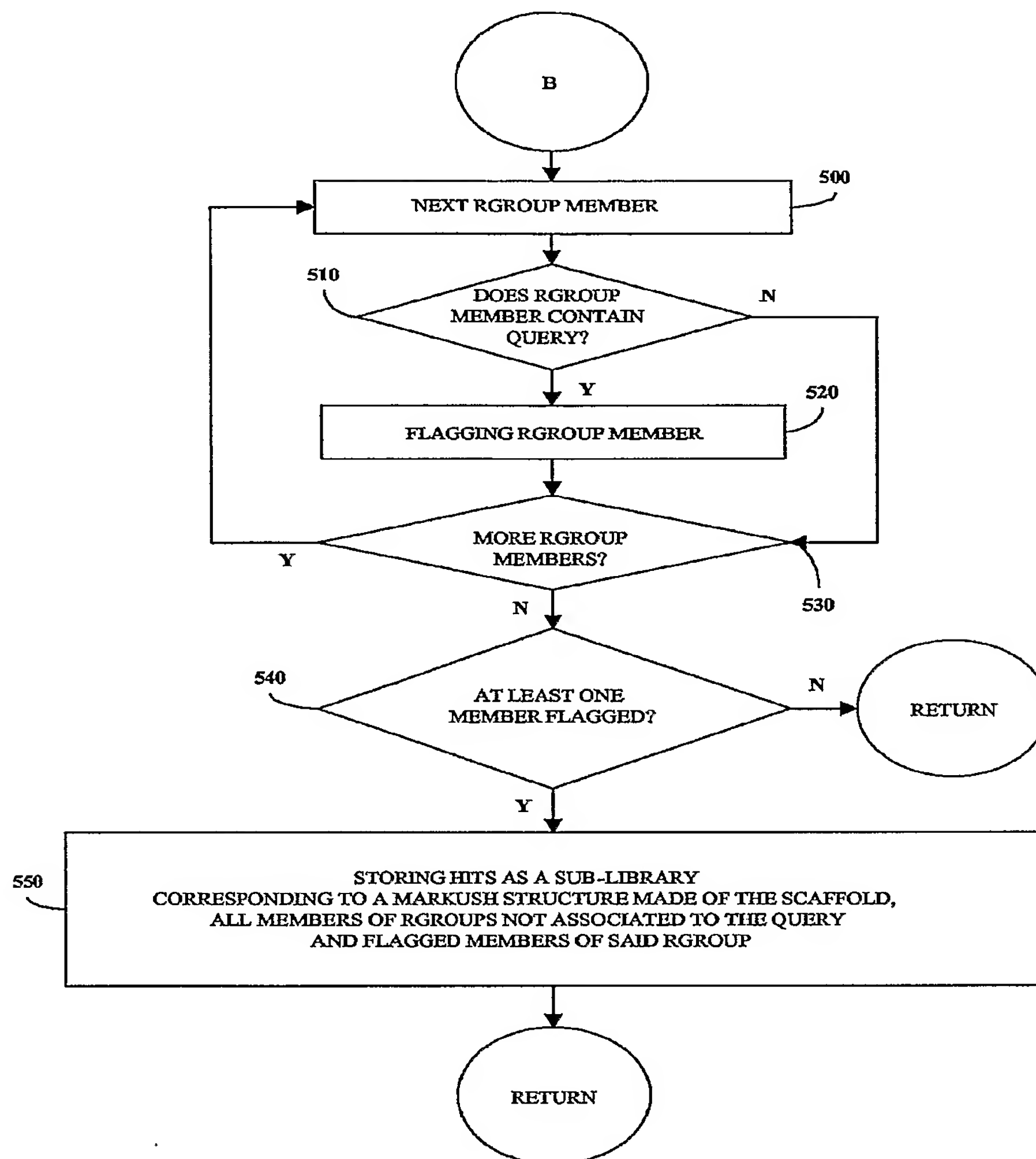
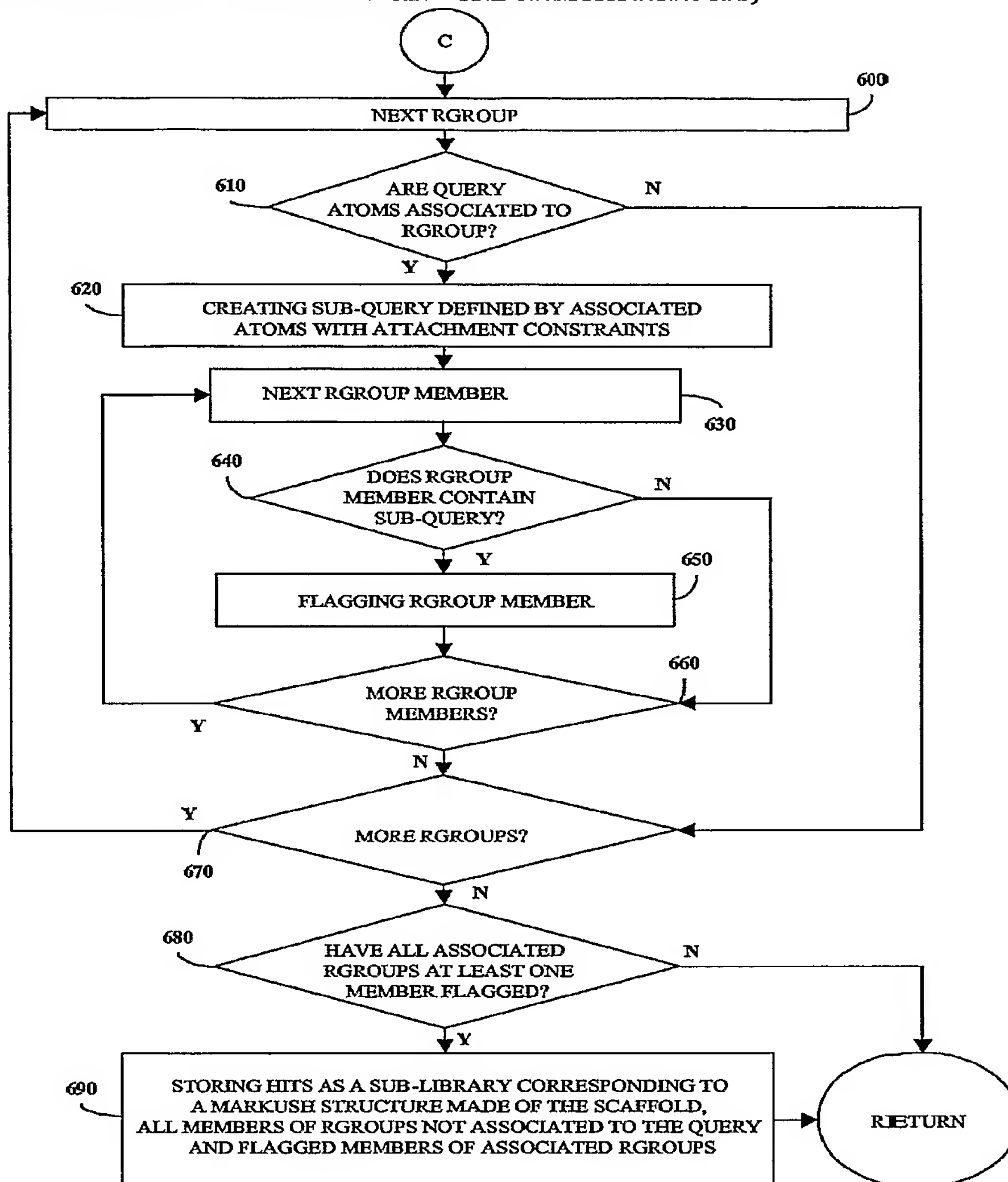


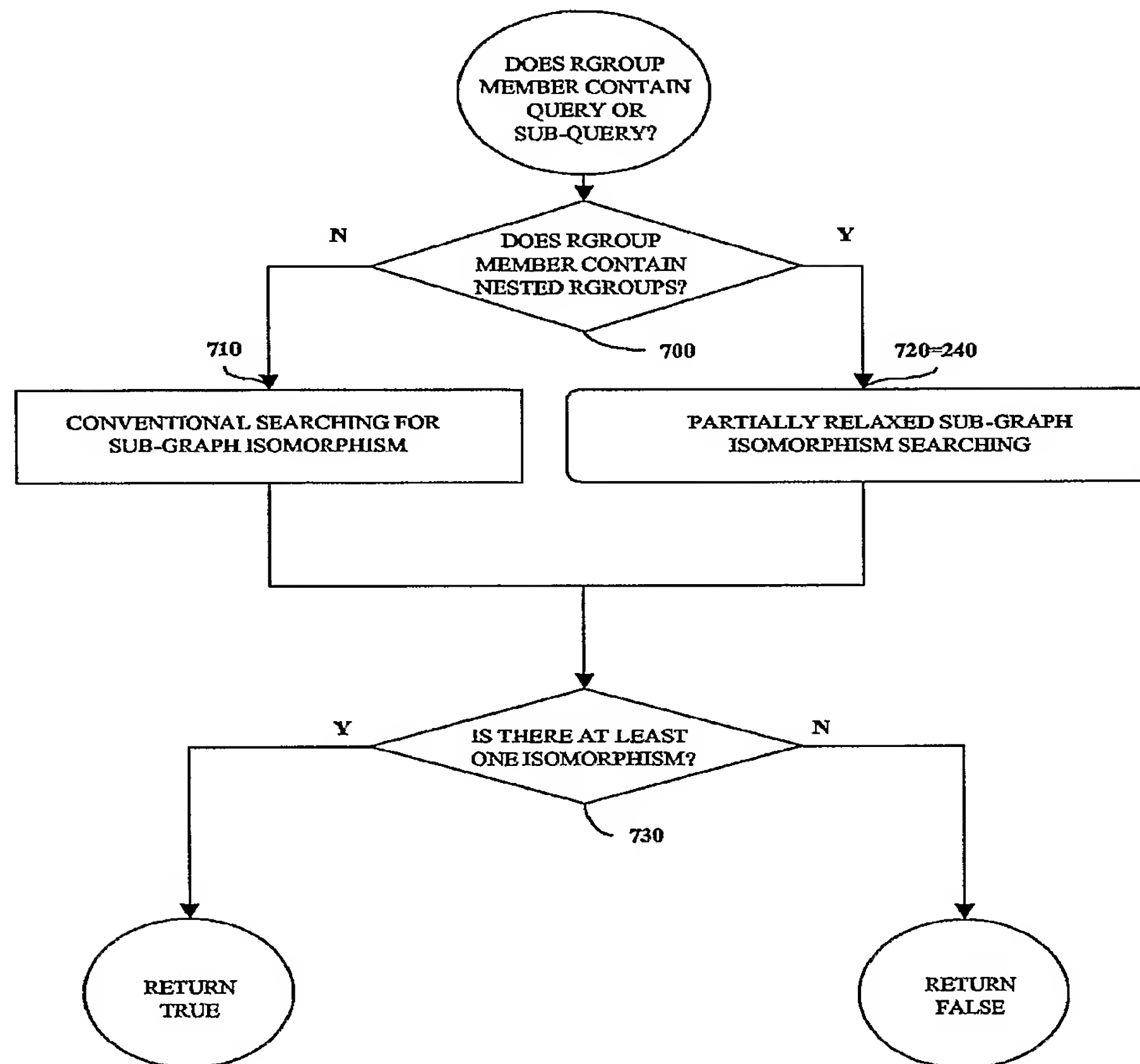
Figure 6

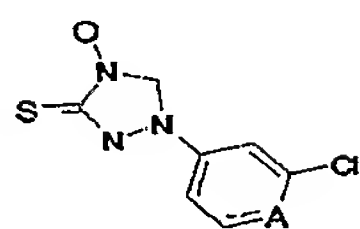
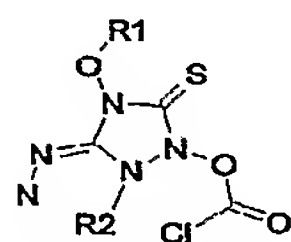
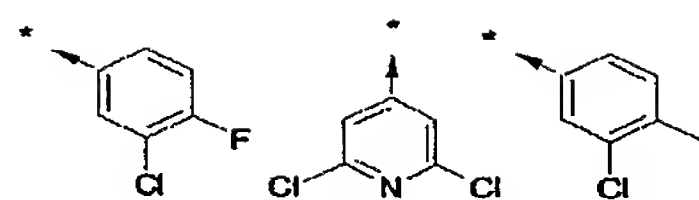
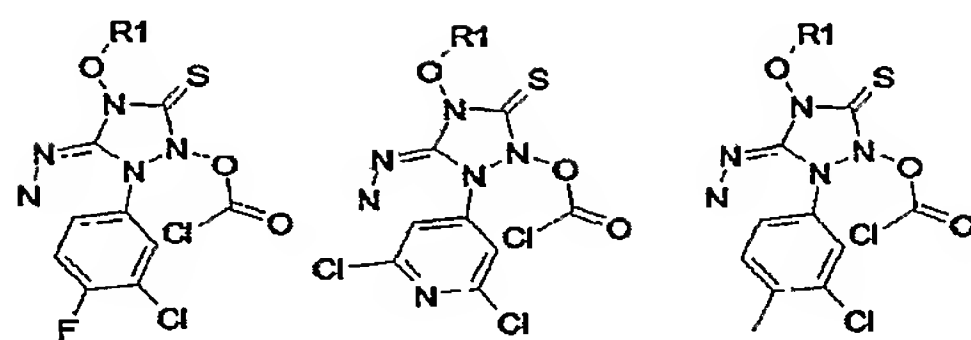
SUBROUTINE:  
C (QUERY SPANS ACROSS THE SCAFFOLD AND ONE OR MORE RGROUPS)



**Figure 7**

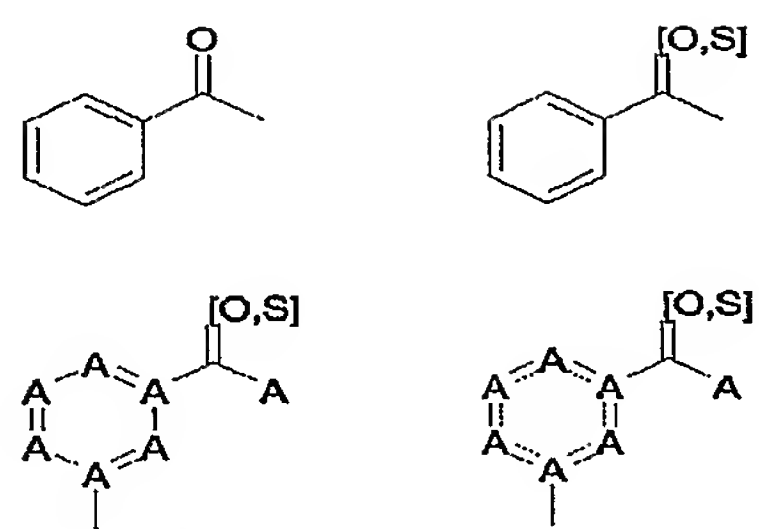
TEST USED IN SUBROUTINES B AND C  
DOES RGROUP MEMBER CONTAIN QUERY OR SUB-QUERY?



**Figure 8****Query structure****Library scaffold****Hits in set R2****Corresponding enumerated hits****Example of search**



**Figure 9**



**Examples of query structures handled by the method**

**Figure 10**

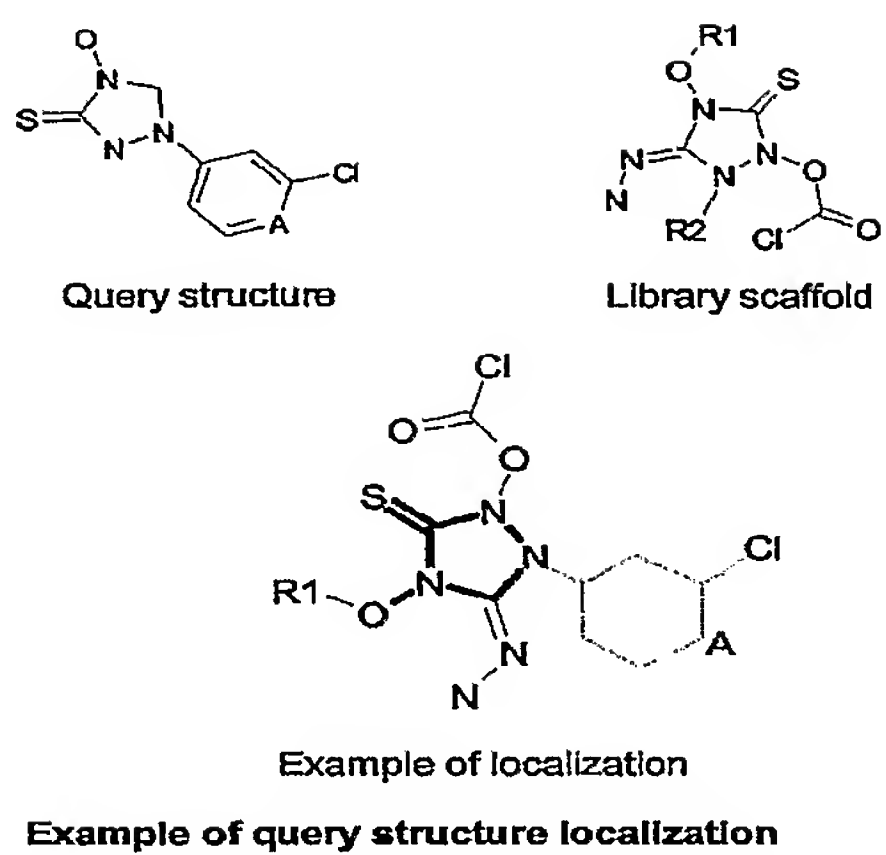
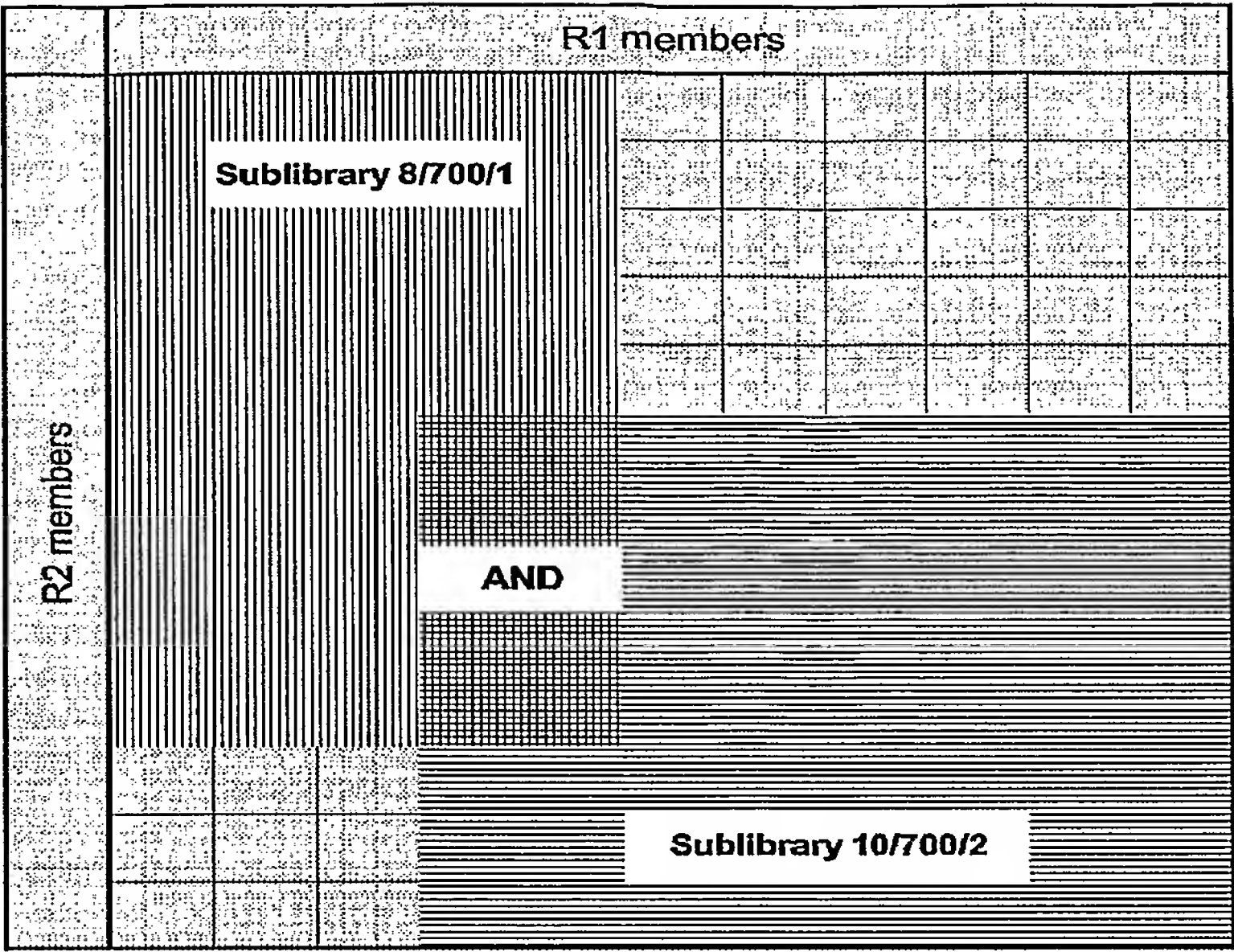
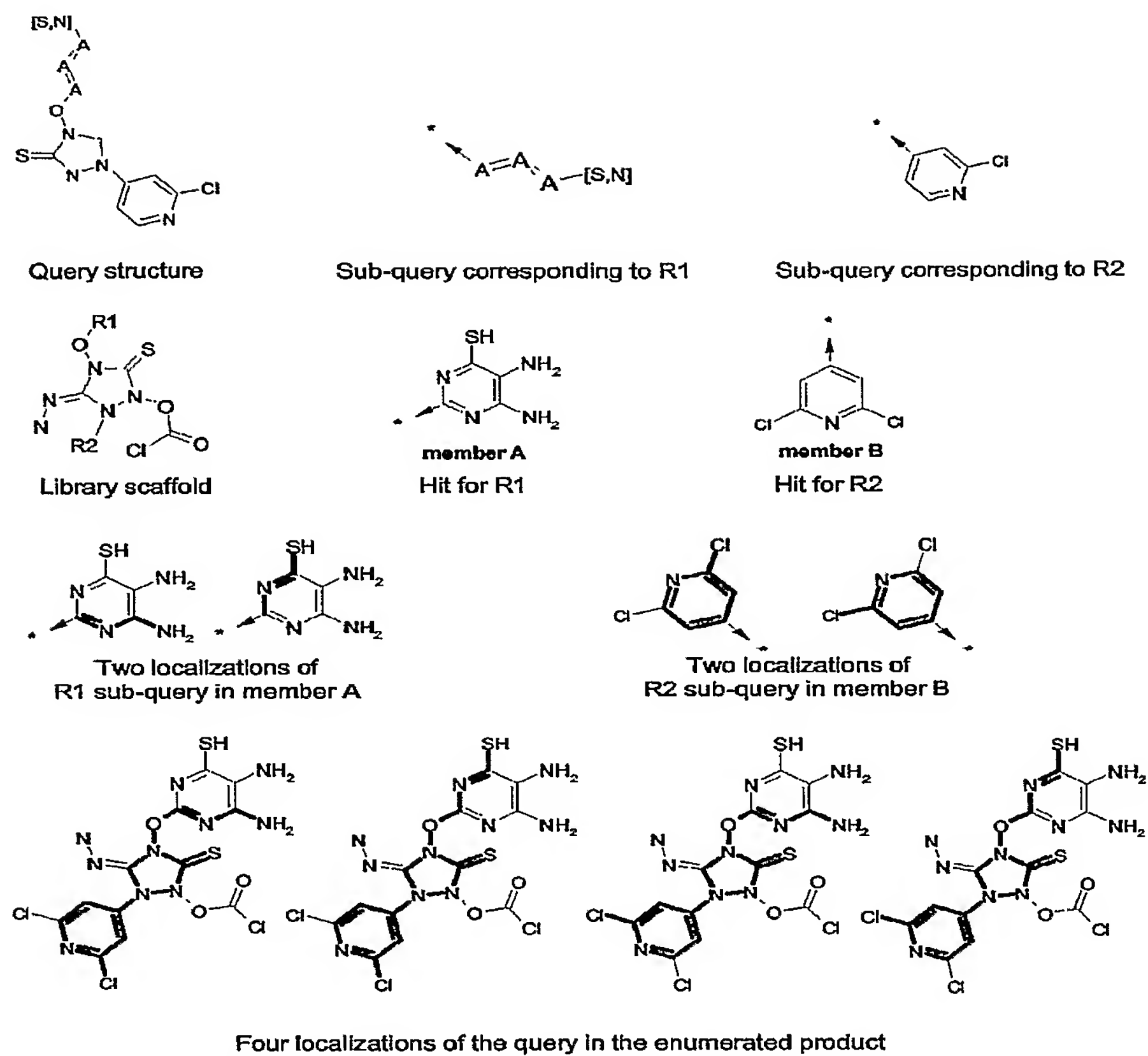


Figure 11



**Figure 12**

**Counting the occurrence of a query structure in compounds for a given isomorphism**



Figure 14

Virtual Combinatorial Library - http://ch78005.spr.astrono.com/VDEV/

File Edit View Favorites Tools Help

Search Favorites History

Address http://ch78005.spr.astrono.com/VDEV/

**VCL** **New query**

Libraries

VCL queries

Prefs

Help

Admin

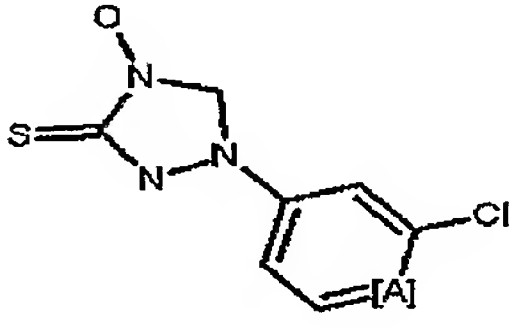
Logout

Name Patentexample

Description Figure 2: example of search

Folder Tests

Substructure



Start search

Done Load dataset

Figure 15

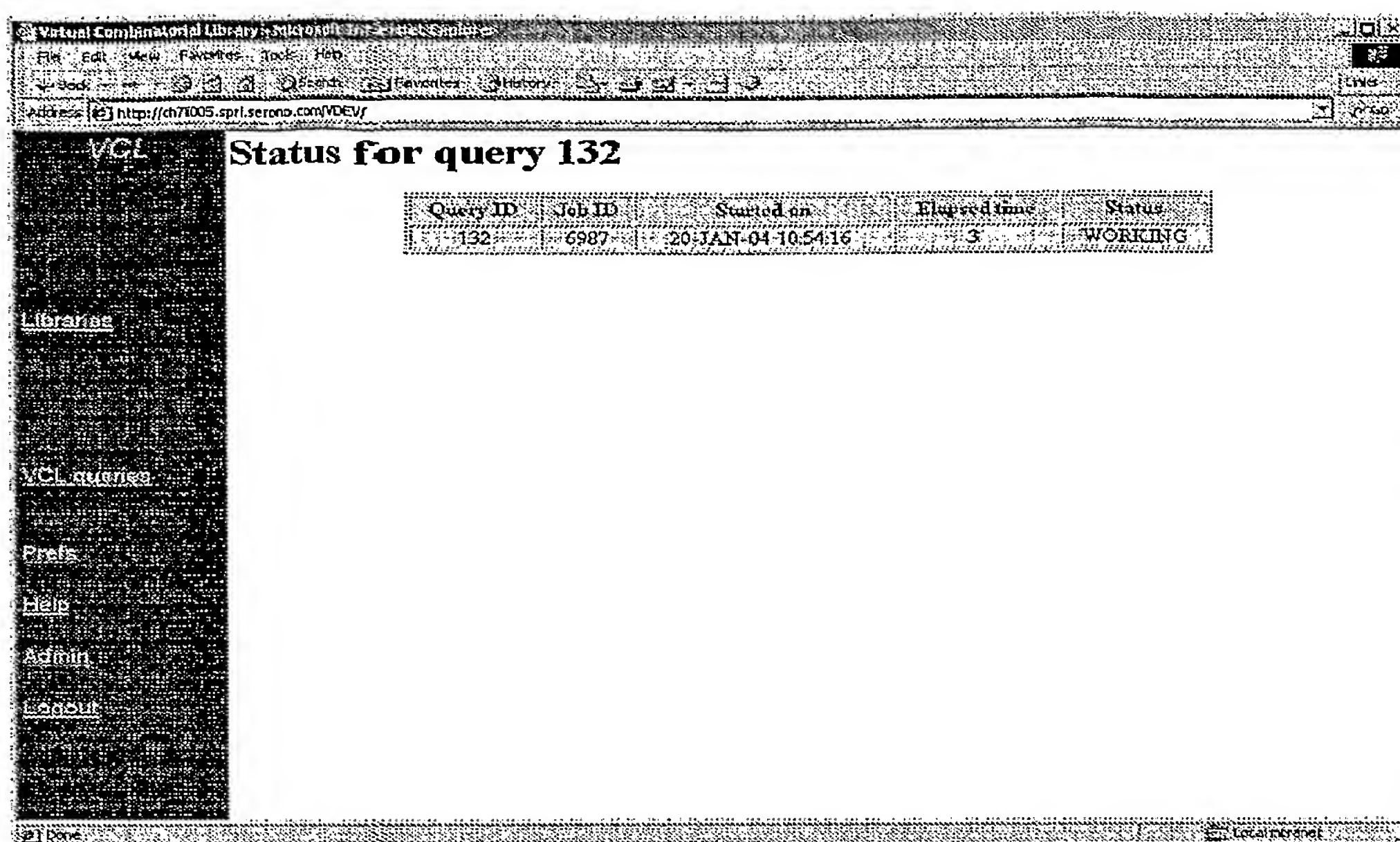




Figure 16

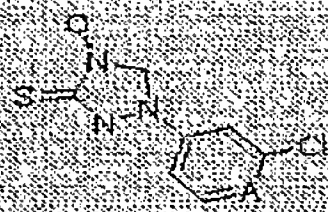
Virtual Combinatorial Library Search Interface

File Edit View Favorites Tools Help

Address: http://d71005.sprl.scrn.com/NDEV/

### Hits for Patent example

Query definition

Name	Patent example
Structure	
Description	Figure 2: example of search
Update	
Last run	20-JAN-04 10:54:16
Status	DONE
Owner	Cedric Mader

Mappings

Sub-library ID	Library name	Map type	R1	R2	Enumerate
132/850/4	CL00001	Spans	Any (171)	3 (172)	Enumerate

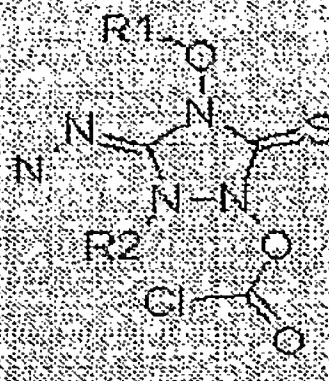
Done



Figure 17

Virtual Combinatorial Library - Microsoft Internet Explorer

## Enumerate hits for 132/880/4



Chemical structure diagram showing a 1,3,4-oxadiazole ring system. The ring is substituted with R1 at position 2, R2 at position 5, and a chlorine atom (Cl) at position 4. The ring is also substituted with a sulfur atom (S) at position 6.

Rgroups to be enumerated:

☐ R1 members

☒ R2 members

[Check involved Rgroups](#)

[Check all Rgroups](#)

☐ Clean structures

☒ Replace RGroups with C atom

Sampling rate

Min samples

Max samples

[Enumerate](#) [Sample](#) [Close](#)



Figure 19

